Nuclear structure: from mean-field to beyond-mean-field calculations

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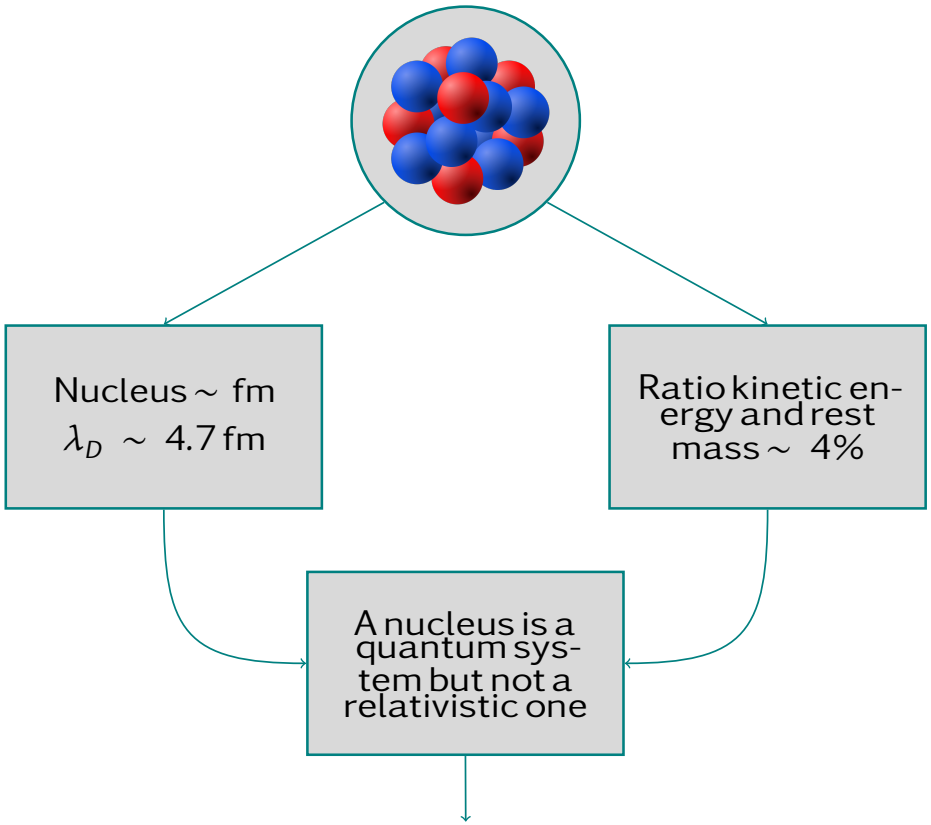
Outline

1. Introduction: what is nuclear structure?
2. Mean-field methods
3. Observables
4. Limitations of the mean-field methods
5. A novel interaction
6. Conclusion

Introduction

Nuclear structure

Study of the static properties of atomic nuclei (size, shape, spectrum, ...)



$$\hat{H}\Psi = \left(\hat{T} + \hat{V}_2 + \hat{V}_3 + \ldots\right)\Psi \, .$$

- Problem: $\Psi = \Psi(x_1, \ldots, x_A)$;
- $\langle\Psi|\Psi\rangle \rightarrow$ integral in $L^2(\mathbb{R}^{3A})$;
- Moreover, the nuclear interaction is not well known ;
- Mean-field: a nucleon undergoes an average potential created by all other nucleons.

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1. Introduction: what is nuclear structure?
2. Mean-field methods
   - Hartree-Fock approximation
   - Effective nuclear interactions
3. Observables
4. Limitations of the mean-field methods
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Hartree-Fock approximation

1. We consider another wavefunction (no correlations, HF only)

$$\Psi \quad \longrightarrow \quad \Phi(x_1,\ldots,x_A) = \frac{1}{\sqrt{A!}} \det[\varphi_{\alpha_1}(x_1)\ldots\varphi_{\alpha_A}(x_A)] \,;$$

   The integral in $L^2(\mathbb{R}^{3A})$ becomes A integrals in $L^2(\mathbb{R}^3)$;

2. We do not provide an expression for the average potential. We construct an effective nucleon-nucleon interaction instead.

- Hartree-Fock (HF) energy

$$E[\rho] = \frac{\hbar^2}{2m}\int \mathrm{d}x\ \tau(x) + \frac{1}{2}\int \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3\mathrm{d}x_4\ v(x_1,x_2;x_3,x_4)\Big[\rho(x_3,x_1)\rho(x_4,x_2) - \rho(x_4,x_1)\rho(x_3,x_2)\Big] \,;$$

- Hartree-Fock equations (+ particle number omitted here)

$$\int \mathrm{d}x_2\ h(x_1,x_2)\varphi_i(x_2) = \varepsilon_i\varphi_i(x_1)\,, \qquad h(x_1,x_2) = \frac{\delta E[\rho]}{\delta\rho(x_2,x_1)}\,.$$

Skyrme interaction

$$v_{Sk}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) \supset \Big[t_0(\mathbb{1}^\sigma + x_0\hat{P}^\sigma) + \frac{1}{2}t_1(\mathbb{1}^\sigma + x_1\hat{P}^\sigma)(\mathbf{k}_{12}^{*2} + \mathbf{k}_{34}^2) + t_2(\mathbb{1}^\sigma + x_2\hat{P}^\sigma)(\mathbf{k}_{12}\cdot\mathbf{k}_{34})\Big]\mathbb{1}^\tau\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})\delta(\mathbf{r}_{12})\,.$$

- Pros:
  1. Fast numerical calculations ;
  2. Easier analytical expressions ;
- Cons:
  1. Functional usually less flexible than finite-range ;
  2. Diverge in HFB.

Gogny interaction

$$v_{Go}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) \supset \sum_{i=1}^{2}(W_i\mathbb{1}^\sigma\mathbb{1}^\tau + B_i\hat{P}^\sigma\mathbb{1}^\tau - H_i\mathbb{1}^\sigma\hat{P}^\tau - M_i\hat{P}^\sigma\hat{P}^\tau)\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})g_{a_i}(\mathbf{r}_{12})\,.$$

- Pros:
  1. Functional usually more flexible than zero-range ;
  2. Does not diverge in HFB ;
- Cons:
  1. Slower numerical calculations ;
  2. More complicated analytical expressions.

- They both contain a density-dependent term

$$\frac{1}{6}t_3(\mathbb{1}^\sigma + \hat{P}^\sigma)\mathbb{1}^\tau\rho_0^\alpha(\mathbf{r}_1)\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})\delta(\mathbf{r}_{12})\,;$$

- Mandatory to reproduce basic properties of nuclei (saturation point, larger effective mass, ...)

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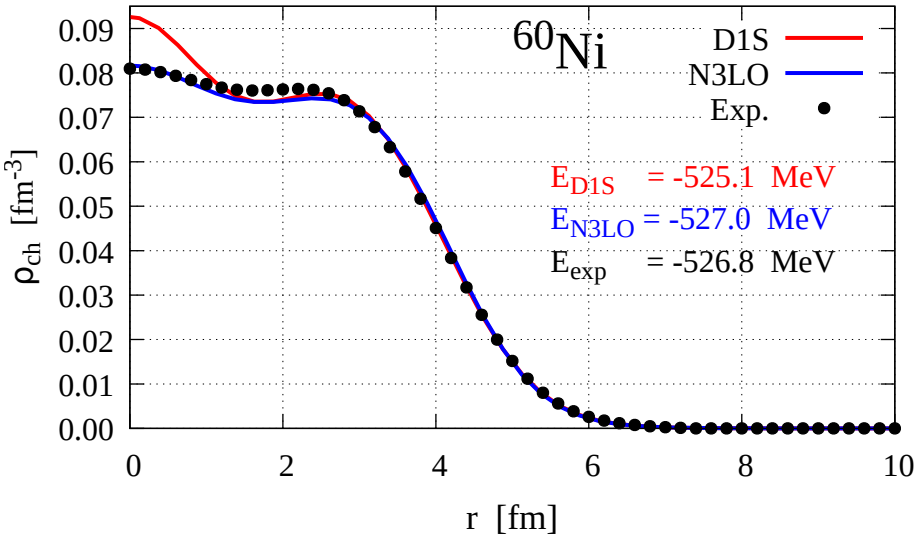
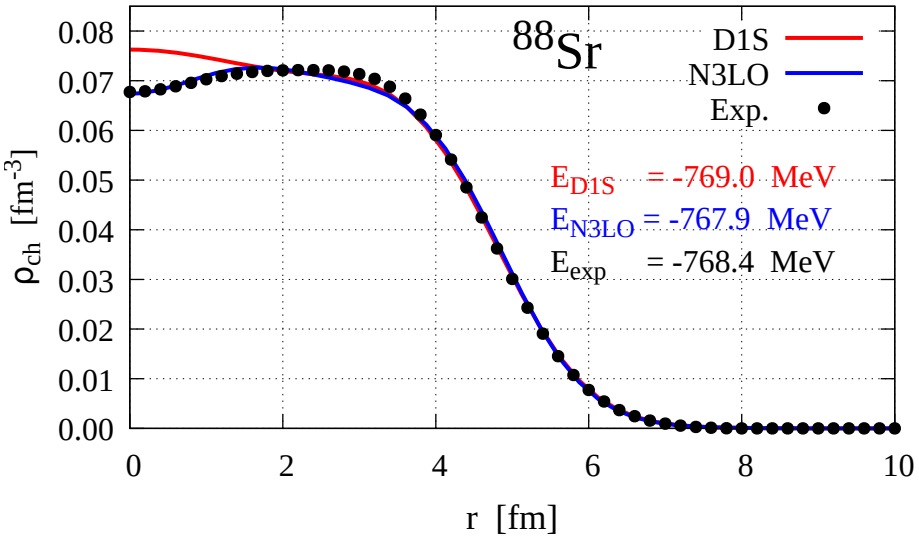
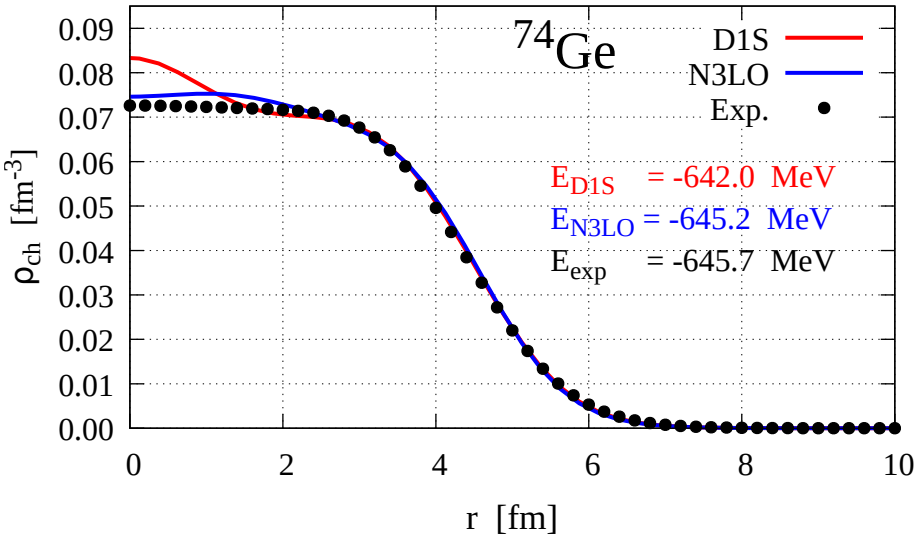
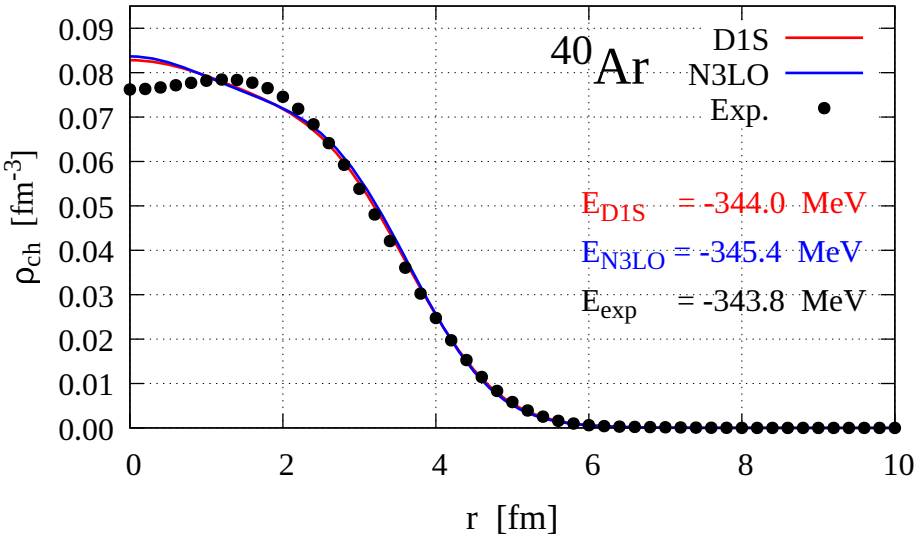
Charge distribution



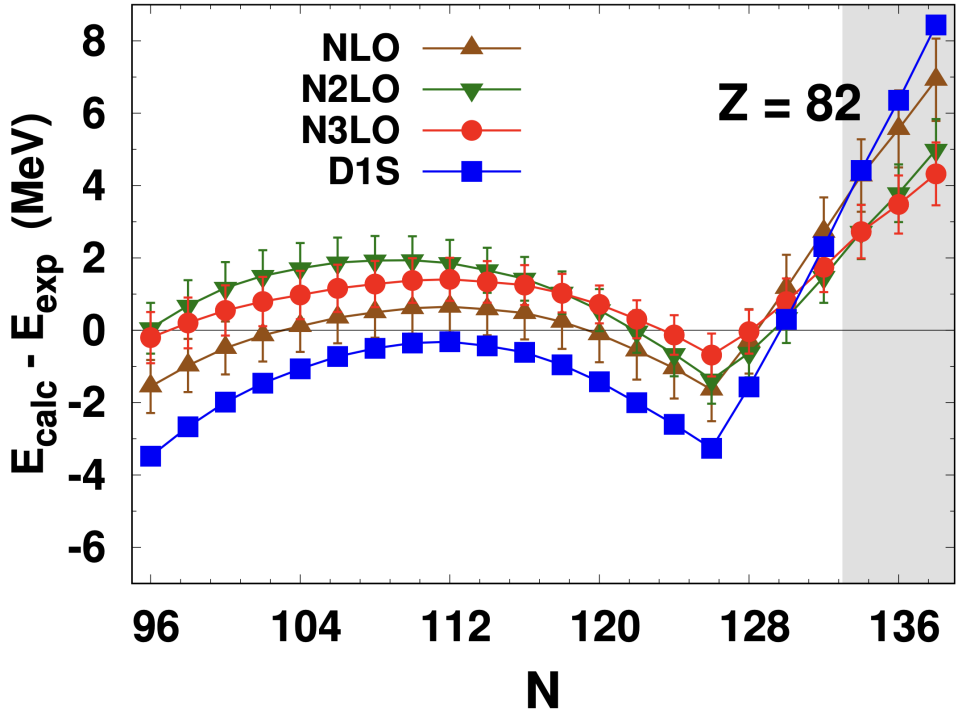


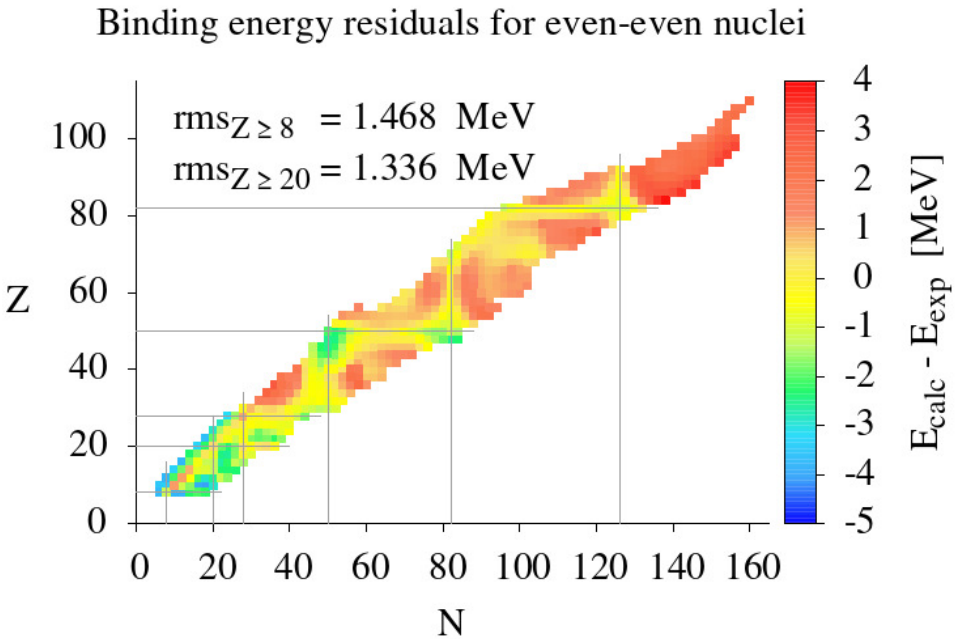




Binding energy

K. Bennaceur *et al.* JPG 47.10 (2020)





Code from M. Kortelainen, HFBTEMP, unpublished

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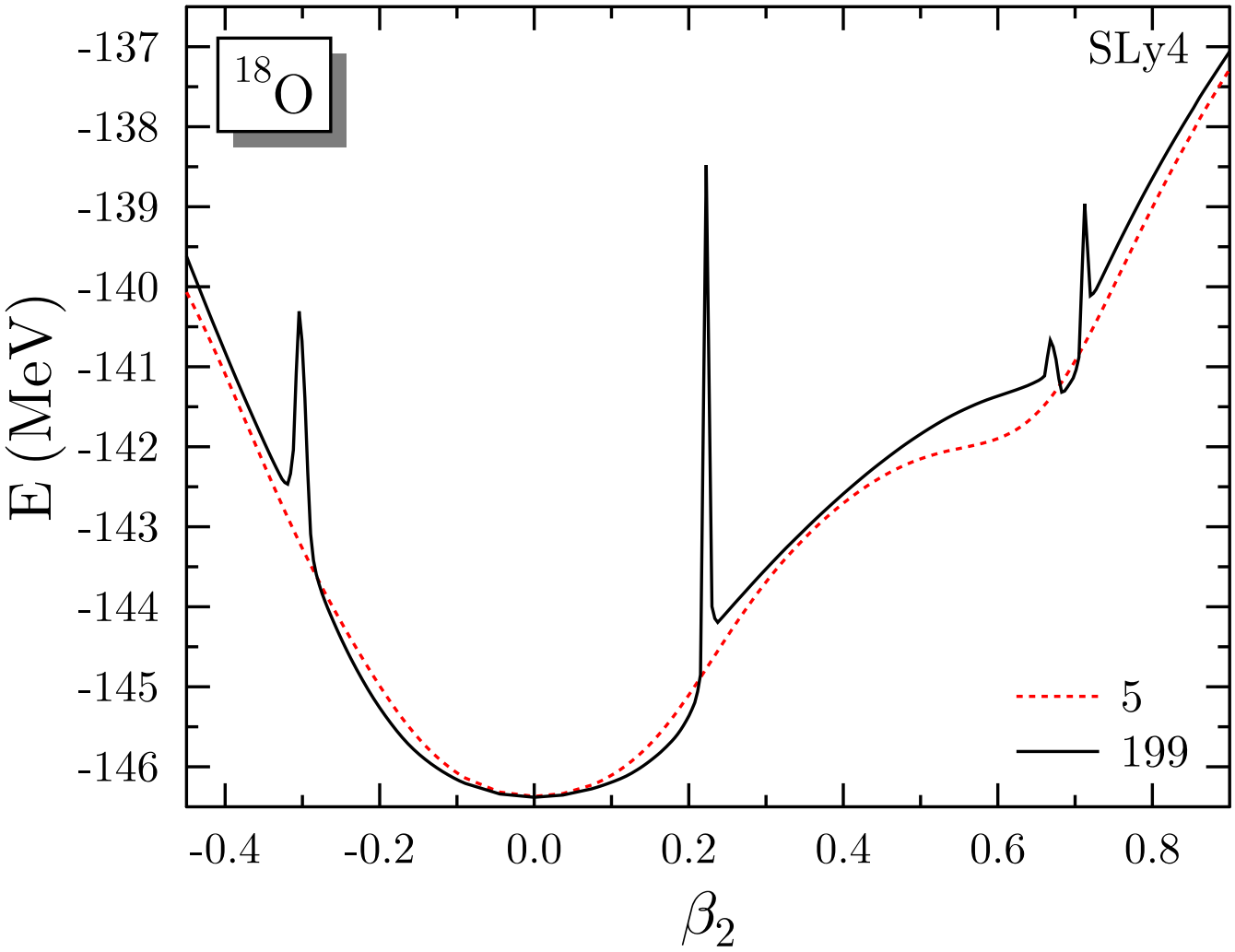

M. Bender *et al.* PRC 78.5 (2008)

There are divergences because:

1. The EDF is not uniquely derived from the underlying potential ;
2. The interaction contains a density-dependent term.

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Three-body semi-regularized interaction

- The most general form (of the central term)

$$\hat{V}^{(n)}_{3,j,bc}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_4,\mathbf{r}_5,\mathbf{r}_6) = W^{(n)}_{3,j,bc}\hat{\mathcal{P}}^{\sigma}_{b}\hat{\mathcal{P}}^{\tau}_{c}\hat{\mathcal{O}}^{(n)}_{j}(\mathbf{k}_{12},\mathbf{k}_{13},\mathbf{k}_{23};\mathbf{k}_{45},\mathbf{k}_{46},\mathbf{k}_{56}) \times \delta(\mathbf{r}_{14})\delta(\mathbf{r}_{25})\delta(\mathbf{r}_{36})\mathcal{G}_a(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{23})\,;$$

- Take

$$\mathcal{G}_a(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{23}) = g_a(\mathbf{r}_{12})\delta(\mathbf{r}_{23}) \qquad \text{and} \qquad \hat{\mathcal{O}}^{(n)}_{j} = \mathbb{1}\,;$$

- Among the 36 EDFs, find which one are linearly independent and hermitian ;
- Remove divergences in the pp channel ;
- In the end, there are two linearly independent functionals and the associated interaction reads

$$\hat{V}_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_4,\mathbf{r}_5,\mathbf{r}_6) = \delta(\mathbf{r}_{14})\delta(\mathbf{r}_{25})\delta(\mathbf{r}_{36}) \times \left\{ W_{3,1}\left(\mathbb{1}^{\sigma} + \hat{P}^{\sigma}_{23}\right) + W_{3,2}\left[\frac{1}{2}\left(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23} + \hat{P}^{\sigma}_{23}\hat{P}^{\sigma}_{12}\right) + \hat{P}^{\sigma}_{12}\right]\right\}\mathbb{1}^{\tau} g_a(\mathbf{r}_{12})\delta(\mathbf{r}_{23})\,.$$

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Conclusion

- Nuclear structure aims at describing the elementary properties of atomic nuclei ;
- Solving the N-body problem is out of reach on today's computers (it will probably never be possible) ;
- Mean-field methods give interesting results for certain observables ;
- However:
  1. They are not predictive enough to extrapolate the results far from the stability ;
  2. They lack the ability of calculating certain observables ;
- We developed an interaction that is usable unambiguously both at the mean-field and beyond-mean-field level ;
- The next step will be to fit the parameters of this interaction to test is predictive power.

Outline

7 Interactions

8 Observables

9 Beyond-mean-field

Two-body effective interaction

- The most general form (of the central term)

$$\hat{V}^{(n)}_{2,j,bc}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = W^{(n)}_{2,j,bc}\hat{P}^{\sigma}_{b}\hat{P}^{\tau}_{c}\hat{O}^{(n)}_{j}(\mathbf{k}_{12},\mathbf{k}_{34})\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})G_a(\mathbf{r}_{12})\,;$$

- The effective interaction is constructed as

$$\hat{V}_2 = \sum_{n,j,b,c} \hat{V}^{(n)}_{2,j,bc}\,;$$

- The values of the parameters W are obtained by minimization of a penalty function.

Three-body pseudo-potential

- The most general form (of the central term)

$$\hat{V}^{(n)}_{3,j,bc}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_4,\mathbf{r}_5,\mathbf{r}_6) = W^{(n)}_{3,j,bc}\hat{\mathcal{P}}^{\sigma}_{b}\hat{\mathcal{P}}^{\tau}_{c}\hat{\mathcal{O}}^{(n)}_{j}(\mathbf{k}_{12},\mathbf{k}_{13},\mathbf{k}_{23};\mathbf{k}_{45},\mathbf{k}_{46},\mathbf{k}_{56}) \times \delta(\mathbf{r}_{14})\delta(\mathbf{r}_{25})\delta(\mathbf{r}_{36})\mathcal{G}_a(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{23})\,;$$

- If $\mathcal{G}_a$ has finite-size in every directions, calculations time might not be tractable ;
- We therefore used

$$\mathcal{G}_a(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{23}) = g_a(\mathbf{r}_{12})\delta(\mathbf{r}_{23})\,;$$

- Additionally, we considered a LO interaction such that

$$\hat{V}_{3,bc}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_4,\mathbf{r}_5,\mathbf{r}_6) = W_{3,bc}\hat{\mathcal{P}}^{\sigma}_{b}\hat{\mathcal{P}}^{\tau}_{c}\delta(\mathbf{r}_{14})\delta(\mathbf{r}_{25})\delta(\mathbf{r}_{36})g_a(\mathbf{r}_{12})\delta(\mathbf{r}_{23})\,.$$

How many operations are needed to evaluate the energy?

- Assume b and c are fixed:

$$4\int, \qquad 6\sum_{\text{spin}}, \qquad 6\sum_{\text{isospin}}, \qquad \rho\rho\rho \rightarrow 4\times 4\times 4 = 64$$

- Total: $4\times 6\times 6\times 64 = 9216$ operations ;
- But the interaction must be symmetrized. Multiply this by $6 \rightarrow 6\times 9216 = 55\ 296$ operations ;
- Now let b and c vary. Multiply this by 36

$$36\times 55\ 296 = 1\ 990\ 656 \text{ operations ;}$$

- Remark: this is only for the particle-hole channel 

Linearly independent functionals

- Fortunately, this number can be reduced:
  1. Some combinations of spin and isospin exchange operators are not hermitian:

     Among the 36 EDF, only 15 are hermitian ;

  2. Some functionals are linearly dependent:

     Among the 36 hermitian EDF, only 9 are linearly independent ;

- We added a constraint to avoid divergences ;
- In the end, we are left with two linearly independent functionals and the associated interaction reads

$$\hat{V}_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_4,\mathbf{r}_5,\mathbf{r}_6) = \delta(\mathbf{r}_{14})\delta(\mathbf{r}_{25})\delta(\mathbf{r}_{36}) \times \left\{ W_{3,1}\left(\mathbb{1}^{\sigma} + \hat{P}^{\sigma}_{23}\right) + W_{3,2}\left[\frac{1}{2}\left(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23} + \hat{P}^{\sigma}_{23}\hat{P}^{\sigma}_{12}\right) + \hat{P}^{\sigma}_{12}\right]\right\} \mathbb{1}^{\tau} g_a(\mathbf{r}_{12})\delta(\mathbf{r}_{23}) \,.$$

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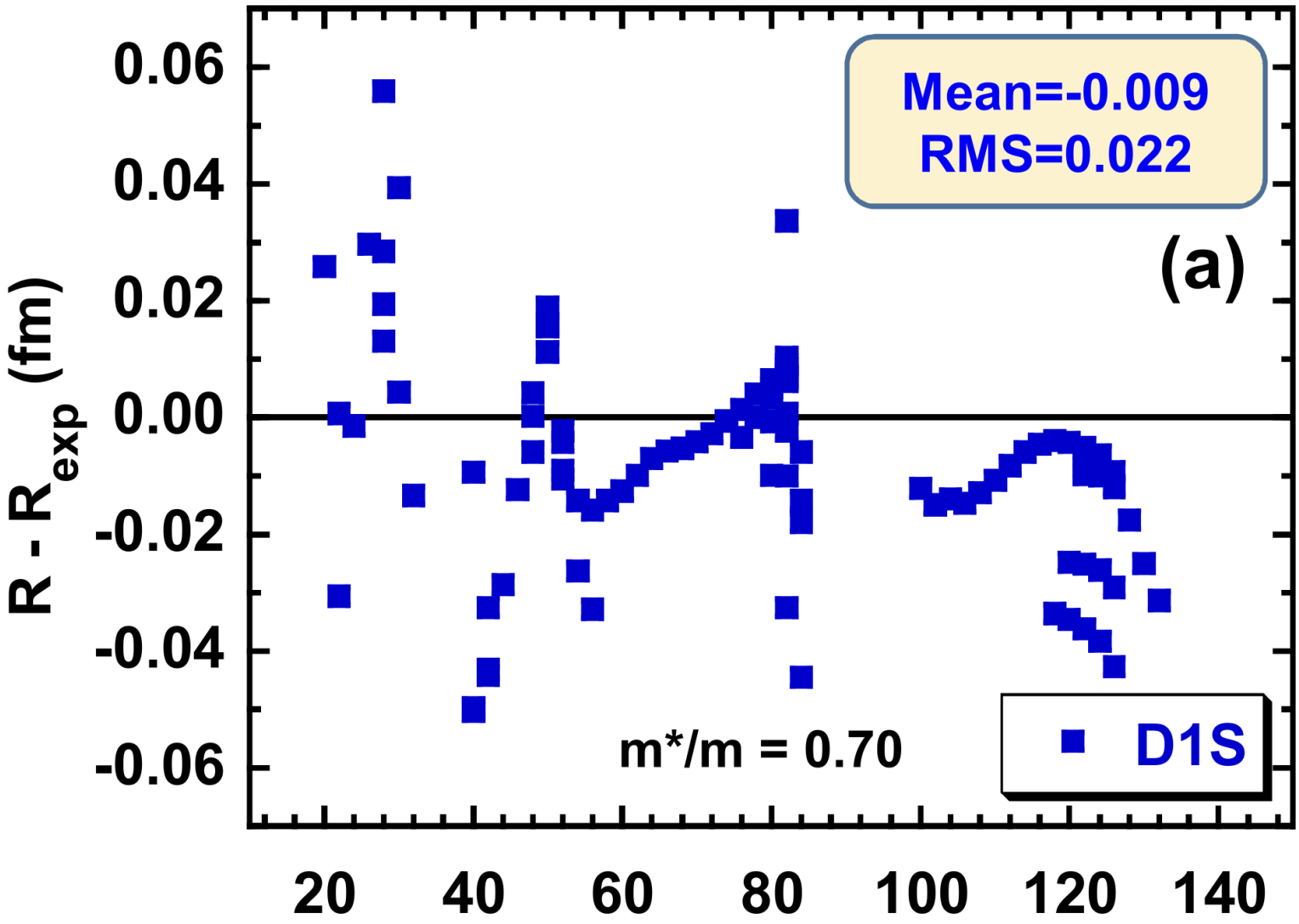
Mean=-0.009
RMS=0.022
(a)
m*/m = 0.70
D1S
R - R_exp (fm)
0.06
0.04
0.02
0.00
-0.02
-0.04
-0.06
20
40
60
80
100
120
140

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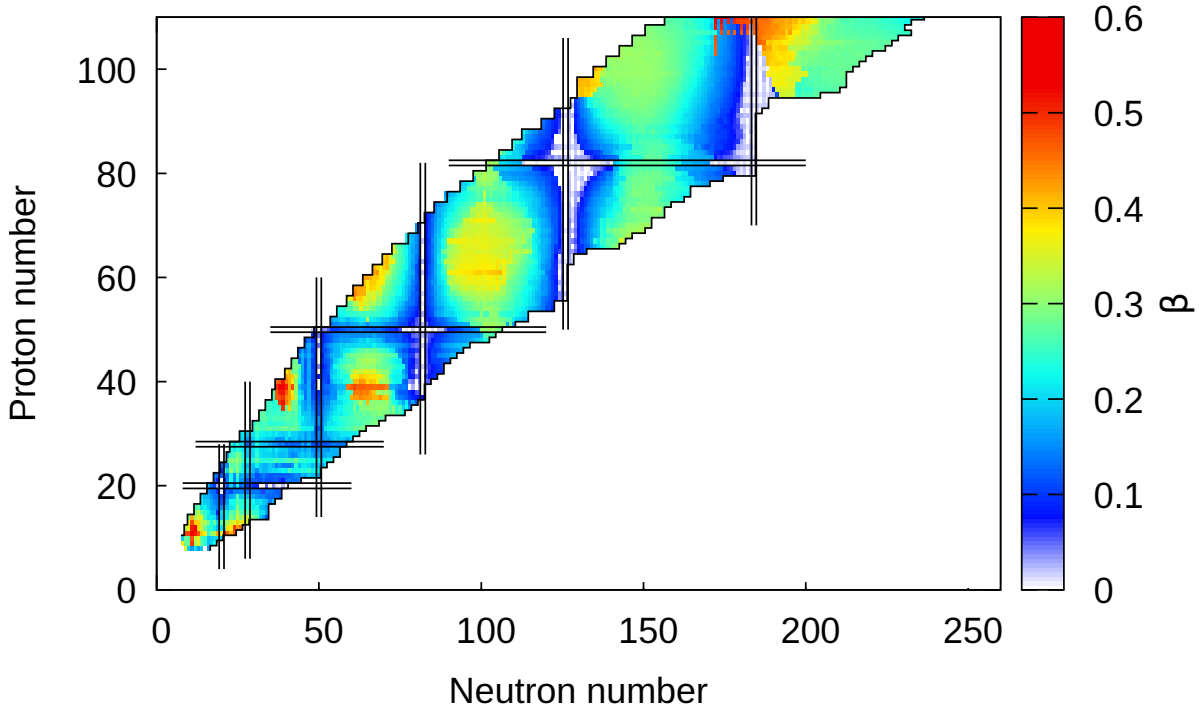
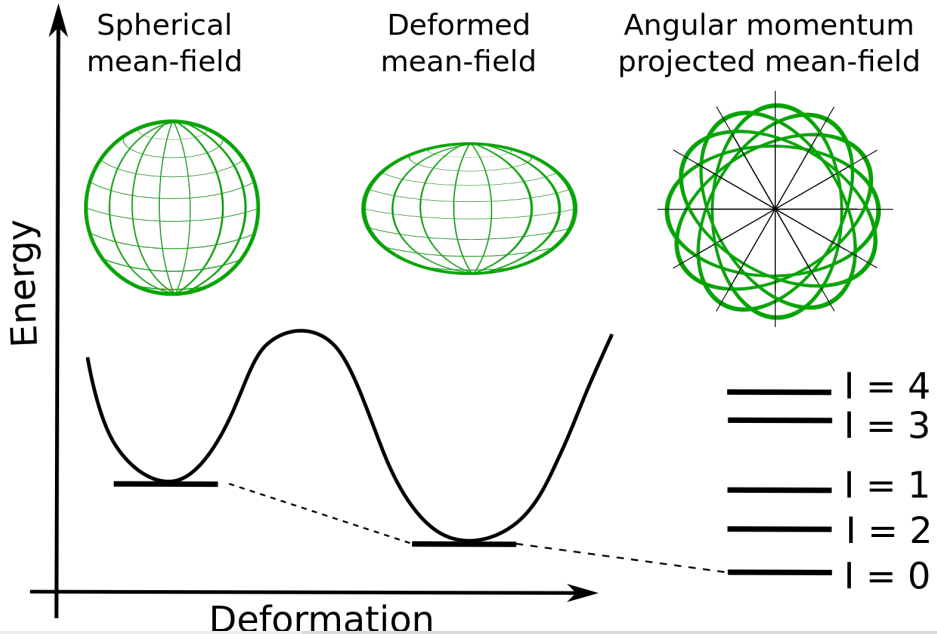
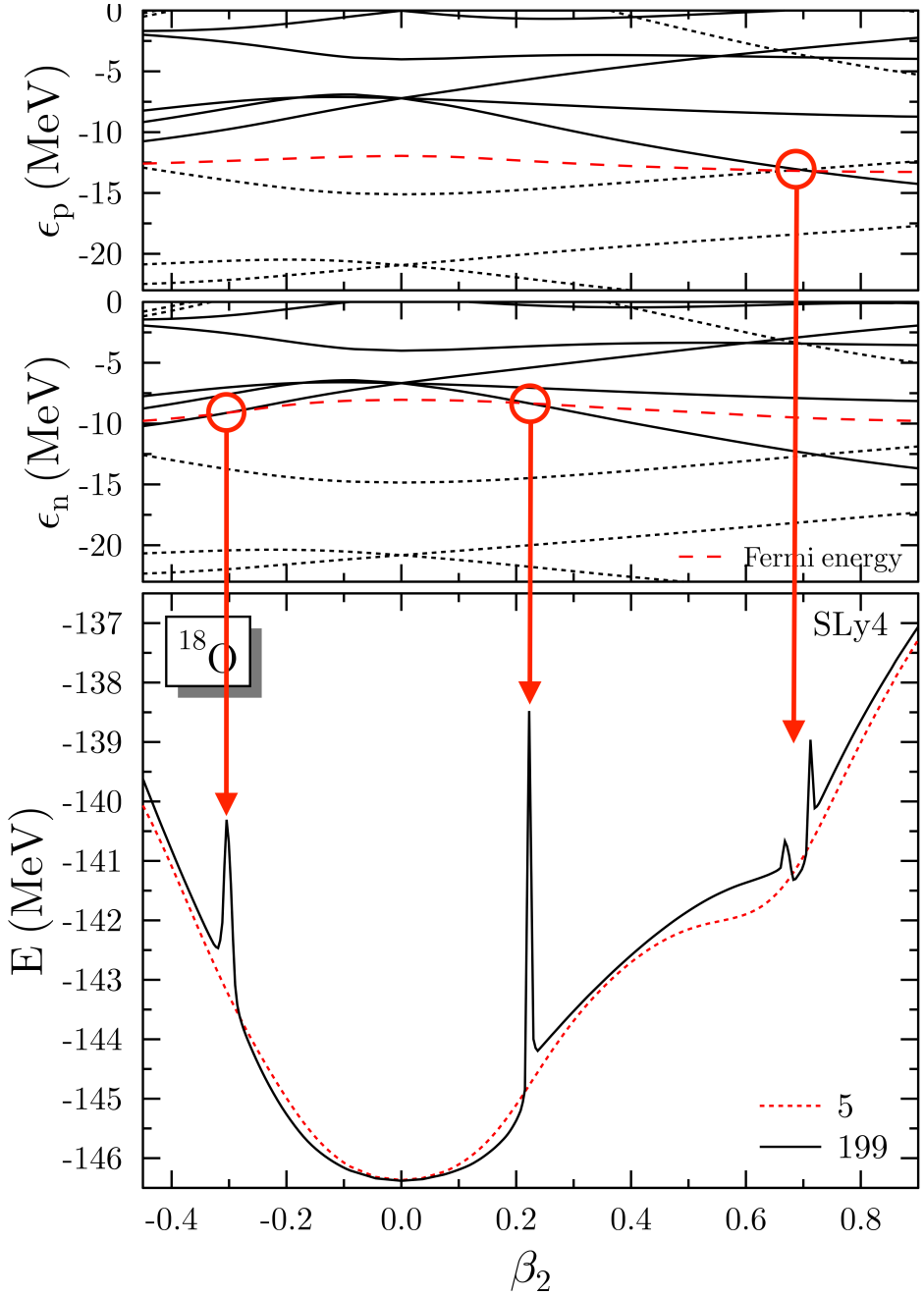
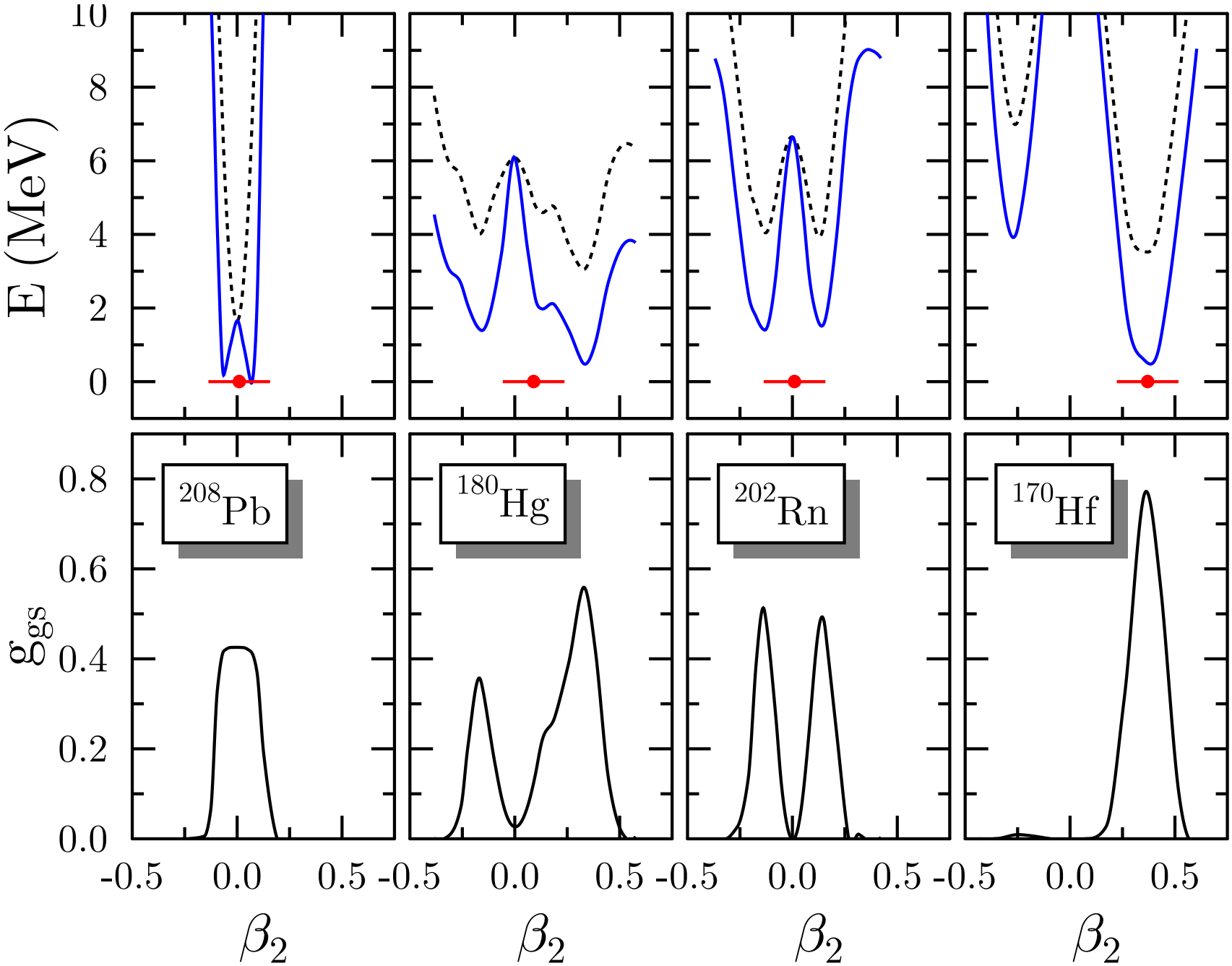


M. Bender *et al.* EPJ A 57.12 (2021)

N. Schunk, Wikimedia common




ϵ_p (MeV)
ϵ_n (MeV)
Fermi energy
^{18}O
SLy4
E (MeV)
5
199
β_2


E (MeV)
10
8
6
4
2
0
^{208}Pb
^{180}Hg
^{202}Rn
^{170}Hf
g_{gs}
0.8
0.6
0.4
0.2
0.0
-0.5
0.0
0.5
β_2